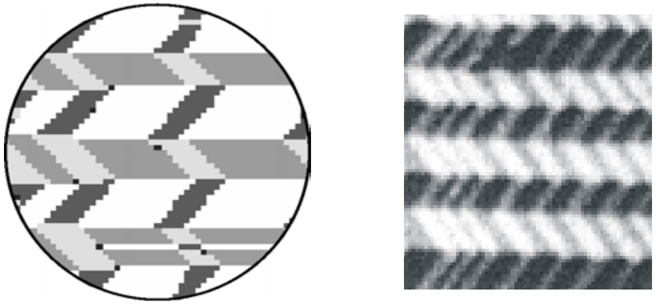
Kinetics of Structural Transformations in Metal and Ceramic Systems

— Martensitic Transformation and Shape Memory Alloys —

Armen G Khachaturyan, Rutgers University, DMR Award #9817235

Martensitic transformation is a displacive crystal lattice rearrangement that produces several orientation domains. A stress-induced domain rearrangement is the underlying mechanism of the shape memory effect and superelasticity. Because of the unique properties of shape memory alloys, they can be used as smart materials and, in particular, as sensors and actuators simultaneously. The computer simulation of martensitic transformation in shape memory alloys is crucial for understanding their thermodynamics and special physical properties.

The three-dimensional computer simulation of martensitic transformation in a single crystal of the important AuCd shape memory alloy predicts the complex self-accommodating pattern of four types of martensitic domains that is in excellent agreement with the experimental observation. The agreement validates a possibility of realistic "virtual experiments" through computer simulation, which can answer the questions that would be difficult or even impossible to be answered in real experiments.



"Virtual experiment" by computer simulation realistically reproduces the complex multi-domain microstructures (left) that is in excellent agreement with the real experimental observation by optical microscopy (right, courtesy of K. Otsuka).

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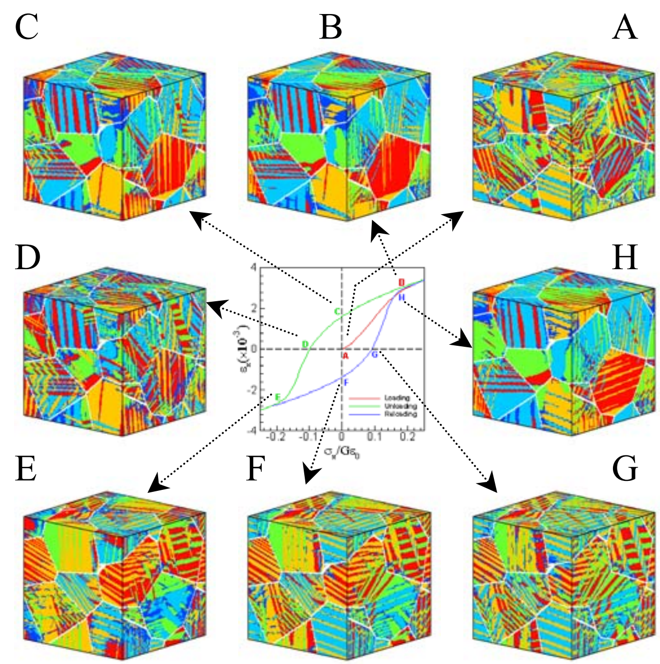
So far there is no answer to a question: how material polycrystallinity affects martensitic transformation and shape memory effect? This is a very important question because most shape memory alloys are polycrystals.

The first computer simulation of martensitic transformation in a polycrystalline shape memory alloy AuCd is shown in the figure. The simulation reveals that the martensitic transformation in a polycrystal and its response to applied stress are significantly different from those in an unconstrained single crystal without pinning defects. The difference is associated with the constraint that is imposed on martensitic transformation by the elastic coupling of neighboring transformed grains with different orientations. The stress-strain hysteresis is associated with the martensitic domain rearrangement under applied stress. The simulated hysteresis curves can be directly used for a formulation of realistic constitutive equations for a larger scale engineering calculations of the functioning of shape memory alloys.



Simulated stress-strain hysteresis curve and the corresponding martensitic domain microstructures.

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— Material Defects and Property Degradation —

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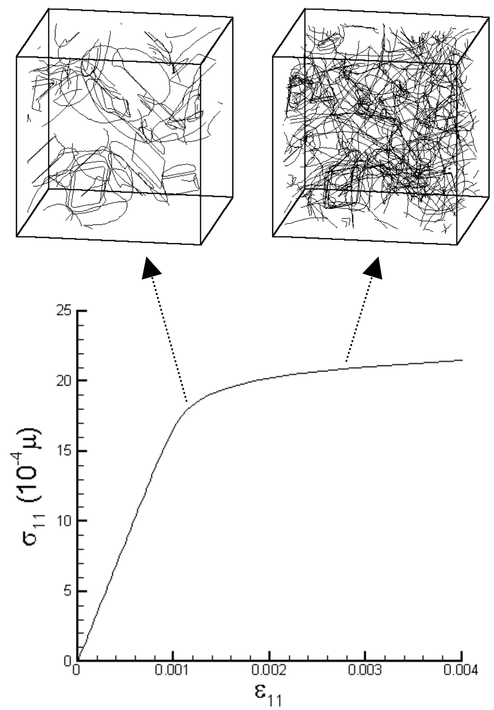
The mesoscopic material defects, such as dislocations, cracks and elastic inhomogeneities, significantly affect the performance of materials. In particular, dislocations reduces the recoverable strain resulting in loss of shape memory effect, and cracks leads shape memory alloys to fracture. Both dislocations and cracks may nucleate upon stress concentration due to elastic inhomogeneities. It is crucial to investigate the effects of material defects on material properties and their degradation.

We developed the Phase Field Microelasticity theory that allows one to realistically prototype plastic deformation and fracture in inhomogeneous materials through three-dimensional computer simulation of evolution of multi-dislocation and multi-crack systems.

The 3-dimensional computer simulation of multi-dislocation dynamics and corresponding stress-strain relation is shown in the figure, where dislocations self-multiply and self-organize under applies stress.



Simulated stress-strain curve associated with multi-dislocation dynamics. Dislocations self-develop from sessile segments by Frank-Read mechanism.

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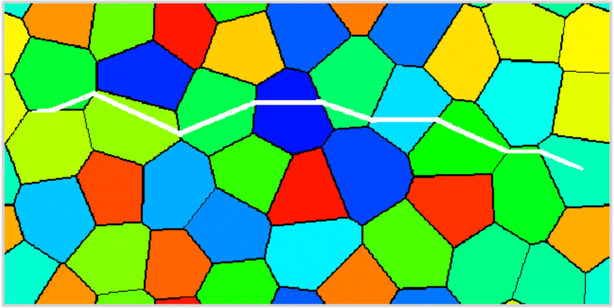
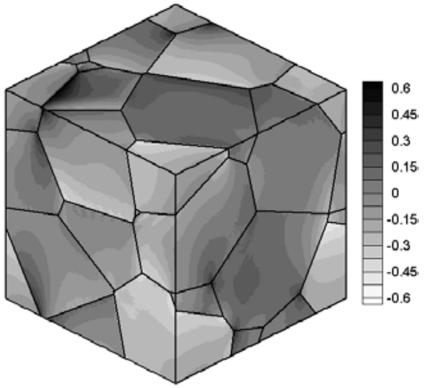
The first Phase Field Theory of crack system evolution is developed. The computer simulations of crack propagation in polycrystal and stress concentration due to elastic inhomogeneity are shown in the figures. Grain boundaries and their junctions are the preferred sites for nucleation of dislocations and cracks.

In spite the distinct natures, the Phase Field Microelasticity theory treats all these defects, dislocations, cracks and elastic inhomogeneities, in a unified manner as it does for martensitic transformation. This allows one to attack the whole spectrum of problems in solid materials, in particular shape memory alloys, by using realistic "virtual experiments".





Computer simulations of crack propagation in polycrystal (top) and heterogeneous stress field due to elastic inhomogeneities in polycrystal comprised of elastically anisotropic grains (bottom).

Education:

2 graduate students (Yongmei M. Jin, Chin-Cheng Su) and 1 postdoctoral research associate (Yu U. Wang) in theoretical and computational materials modeling have participated in this research.